"PICOSECOND DIELECTRIC RELAXATION STUDIES OF MONOHYDRIC, DIHYDRIC AND TRIHYDRIC ALCOHOLS"

Synopsis

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Research proposal submitted
In partial fulfillment of registration to
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By

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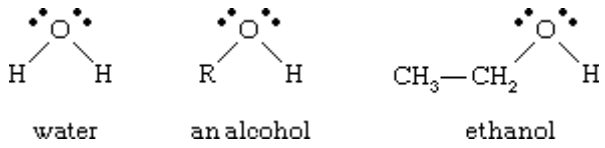
Abstract of proposed work plan/problem

"PICOSECOND DIELECTRIC RELAXATION STUDIES OF MONOHYDRIC, DIHYDRIC AND TRIHYDRIC ALCOHOLS"

1. Introduction

Alcohol is the most popular material employed to study hydrogen-bonding molecular liquids[1-3]. Intermolecular hydrogen bonds can be formed by alcohol molecules, which are seen as organic radicals with attached hydroxyl groups and are highly miscible in water [4]. Alcohols are organic compounds whose molecules contain one or more (–OH) hydroxyl groups attached to a carbon atom characterized by one, two, or three hydroxyl groups. Alcohols may be considered organic derivatives of water (H_2O) in which one of the hydrogen atoms has been replaced by an alkyl group, typically represented by R in organic structures. For example, inethanol (or ethyl alcohol) the alkyl group is the ethyl group, —CH_2CH_3.



water an alcohol ethanol

Most alcohols are colorless liquids or solids at room temperature. Alcohols have low molecular weight and are highly soluble in water; with increasing molecular weight, they become less soluble in water, and their boiling point, vapor, densities, and viscosities increase. Alcohols are classified on the basis of a number of hydroxyl groups present in the structure, they are classified as monohydric dihydric and polyhydric alcohols. The

monohydric alcohols are classified as primary, secondary or tertiary according to which carbon of the alkyl group is bonded to the hydroxyl group.

I. The primary carbon atom of the (−OH) hydroxyl group has attached only one single alkyl group like, ethanol-CH_3– CH_2-OH, propanol-CH_3-CH_2-CH_2-OH, etc.

II. The secondary carbon atom of a hydroxyl group (-OH) is attached to the "two alkyl" group on either side, the two alkyl groups present may be either structurally identical or even different eg. Isopropanol, propan-2-ol, Butan-2-ol, pen-3-ol.

III. The tertiary alcohols are those which feature a hydroxyl group attached to a carbon atom which is connected to the3-alkyl group like tert-butanol.

Dihydric alcohols can be divided into four categories based on where the hydroxyl groups are located. These groups are 12-diol, EN-diol, EE-diol, and NN-diol. Their general formula is $C_nH_{2n+2}O_2$. The simplest and most important dihydric alcohol is ethylene glycol. Trihydric alcohols contain three hydroxyl groups attached to an aliphatic carbon chain eg.Glycerol,1,2,4-butanediol,and 1,2,6-hexanediol.

The objective of the present work is to report the broadband dielectric data of monohydric dihydric and trihydric alcohols, over the wide frequency range. Dielectric spectroscopy provides further insights into the reorientation dynamics of the alcohols [5-6]. This method records the response of polar molecules to an applied oscillating electric field in the form of dielectric loss and dispersion functions which result from the reorientation of molecular dipoles. The dielectric study of materials provides vital information about dielectric parameters and molecular interaction, which are of direct technological importance. The

knowledge of dielectric properties of materials and their frequency and temperature dependence is of great importance in various areas of science and engineering in both basic and applied research. Dielectric properties obtain can be related to a physical parameter of interest. It has been demonstrated that properties such as moisture control, bacterial content, mechanical stress, and other seemingly unrelated parameters are related to the dielectric properties or permittivity of the material. Dielectric relaxation spectroscopy is one of the technique which gives information about dielectric materials. When electrical energy may be stored in dielectrics, which are insulators. When these materials become subjected to an external field, their positive and negative charges shift in the opposite direction, causing the molecules to produce a net dipole moment. This is called polarization of the material and such materials are called dielectrics. The dielectric material becomes polarized when an electric field is applied across it, and the electric field remains inside of them. The molecules are orientated in parallel or anti-parallel orientations depending on the intensity of the applied electric field, the molecular structure, and the kind of bonding[7-10].

2. Literature Review and Development in the Subject (previous work done in the relevant area)

Dielectric relaxation spectroscopy is one of the most popular spectroscopy having frequency range from 10^{-4}Hz to 10^{12}Hz. So, this spectroscopy is known as broad band dielectric spectroscopy [11-16]. The associating behavior of alcohols in aqueous and non-aqueous solution is extensively studied through the dielectric properties, heterogeneous interactions and cooperative domains (CD) [11-12]. In last few decades, considerable experimental and theoretical studies have been reported on the dielectric relaxation behavior of alcohols in polar and non-polar solvent [13-20]. Sudo *et.al*. [17-18] have studied the dielectric relaxation

time and relaxation time distribution in alcohol-water mixtures at room temperature in the frequency range 10 MHz to 20 GHz to understand the correlation between the broadness of dielectric loss peak and the number of carbon atom in alcohol molecule. Sengwa *et. al.* [19-20] studied the comparative dielectric study of mono, di and trihydric alcohols in the frequency range from 10MHz to 20GHz at 25^0C to understand the effect of number of carbon atoms and hydroxyl groups on the dielectric properties. Present work is devoted to study the structural and dielectric relaxation in alcohols.

3. Objective of research/Proposed Hypothesis:

The main objective of the present work is to study

(i) To study the high frequency complex permittivity spectra of various alcohol (mono, di, trihydric).

(ii) To study the dielectric relaxation behaviour of alcohols in presence of polar and non-polar solvent by using time domain reflectometry.

(iii) To study the orientation of electric dipoles in alcohol solution by using the Kirkwood correlation factor.

(iv) To study the Thermodynamic behaviour of systems by using dielectric relaxation spectroscopy technique.

(v) To study the intermolecular interaction in the mixture by using the Bruggeman factor and hydrogen bonded theoretical model.

4. Methodology to be adopted:

The time domain reflectometry (TDR) approach will be used to acquire complex dielectric permittivity spectra. For time domain reflectometry (TDR), the Tektronix DSA8300 Digital

Serial Analyzer sampling mainframe oscilloscope along with sampling module 80E10B will be used. Figure 1 shows experimental setup for TDR [21-22]. A repetitive fast rising 250mVvoltage pulse of 200 KHz with 12ps incident and 15ps reflected rise time was fed through coaxial line system of impedance 50 ohm. Sampling oscilloscope monitors changes in step pulse after reflection from the end of Transmission coaxial line. Reflected pulse without sample $R_1(t)$ and with sample $R_x(t)$ will be recorded in time window of 5ns and digitized in2000 points [23]. Further, the time domain data will be converted to frequency domain using Fourier transformation.

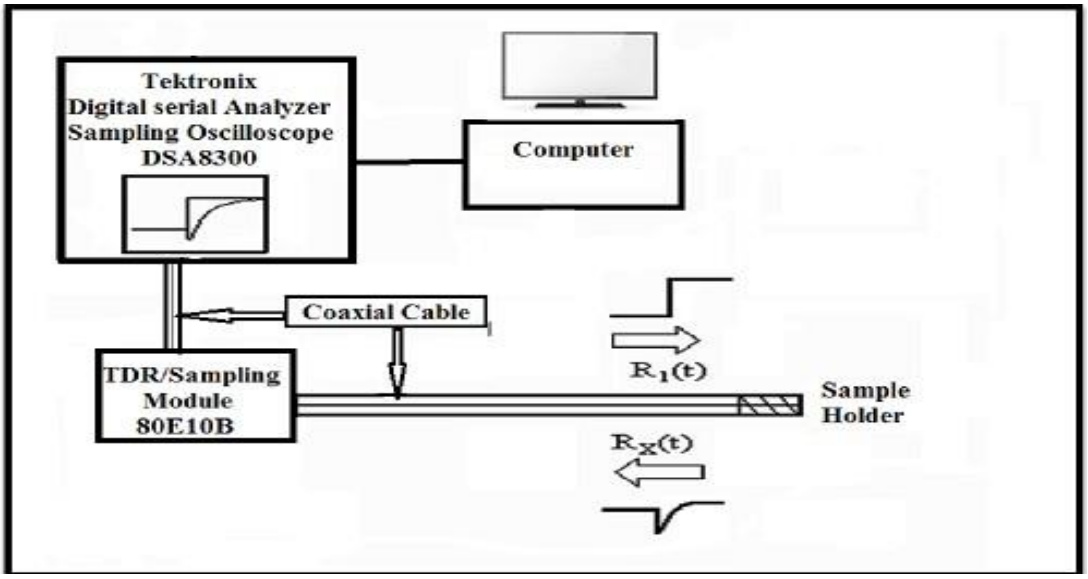


Fig1. Block diagram of Time Domain Reflectometry.

5. Importance of study/society application

Alcohols has widely used in pharmaceutical and medical applications. Alcohols are also used as solvent in various chemical industries. Over the last few decades dielectric

relaxation spectroscopy playing a very important role in understanding the molecular interaction, electric dipole orientation in liquid structure. Therefore it is very important to study their dielectric relaxation behavior to understand the intermolecular interaction in poly alcohols mixtures.

- **International/National status**: T he following scientists are currently working in field of dielectric relaxation spectroscopy at international/national level:

1. F.F. Hanna, Microwave Physics Department, National Research Centre, El-Tahrir St., Dokki, 12311 Cairo, Egypt.
2. V.I. Zhuravlev, Chemistry Department, Moscow State University, Moscow, Russia.
3. A.G. Gilani, Department of Chemistry, Faculty of Science, University of Guilan,41335 Rasht, Iran.
4. V.A. Rana, Department of Physics, Gujrat University, Ahmedabad (Gujrat).
5. R.J. Sengwa, Department of Physics, JNV University, Jodhpur(RS).

- **Significance of the study:**

The evaluated dielectric parameters are used to discuss the change in the shape of dielectric dispersion with increase in hydroxyl groups in the molecular structure of primary alcohols to the polyhydric alcohols. Further, the dielectric parameters are also used to explore the molecular dynamic of intermolecular hydrogen-bonded species and the hindrance to intermolecular rotations in these alcohols. Even though a complete theoretical understanding of the motional processes is not yet achieved, valuable information can be gathered by comparative dielectric studies of alcohols since in this large class of chemically related compounds the interaction determining the association dynamics is in

all cases essentially the same, namely hydrogen bonding between the hydroxy groups. Thus, for example, the influence of steric requirements on association can be studied. Since alcohols have an important role in various chemical land medical industries.

6. Proposed work plan/Formulation and structure of study:

First Year:

(i) Literature survey related to the Thesis topic

(ii) Course Work as per university syllabus

(iii) Literature Review system to be studied.

Second Year:

(i) Measurement and Training for Dielectric and spectroscopic Technique and analysis of dielectric data.

(ii) Extract the dielectric parameters

Third year:

(i) Experimental data will be analyzed

(ii) Present data in International/National Conferences

(iii) Published in different International/National Journals.

(iv) Published experimental data in the peer Reviewed Journals

(v) Writing Thesis and submit to university.

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